Error Bounds for Compound Quadrature of Weakly Singular Integrals

by

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1. Introduction.

The primary purpose of this paper is to develop and analyze some practical numerical methods for handling weakly singular quadrature; that is, for $\int_I f(t)dt$ where f is Lebesgue integrable on I (so called "improper integrals"). We also extend this development and analysis to the case where some derivative of f is Lebesgue integrable and has finitely many unbounded points on I. We shall be particularly interested in obtaining "best" possible order estimates for compound quadratures.

It is known (although possibly not well known) that Peano's theorem can be applied to analyze the error in "low continuity" numerical quadrature. For example $\int_0^T t^{1/2}dt$ approximated by the trapezoid rule:

Let $h > 0$, $Nh = T$, $E(T)$ = error. Then

$$E(T) = \int_0^T t^{1/2}dt - h\{\sqrt{h} + \sqrt{2h} + \ldots + \sqrt{(N-1)h} + (1/2)\sqrt{Nh}\}.$$

By Peano's theorem, c.f. e.g. Sard [1, p. 14]

$$E(T) = \int_0^T (1/2)t^{-1/2}K(t)dt$$

where $K(t) = (j + 1/2)h-t$ on $jh \leq t < (j+1)h$. Apply the Minkowski inequality with $1/p + 1/q = 1$ and $1 \leq q < 2$:

$$|E(T)| \leq (1/2)\{\int_0^T |t^{-1/2}|^q dt\}^{1/q}\{\int_0^T |K(t)|^p dt\}^{1/p}.$$

(Clearly $|t^{-1/2}|^q$ is integrable for $1 \leq q < 2$.) Now use the definition of $K(t)$:

$$\int_0^T |K(t)|^p dt = N \int_0^h |h/2 - t|^p dt = 2N \int_0^{h/2} t^p dt$$

$$= (2N/(p+1))(h/2)^{p+1} = (hN/(p+1))(h/2)^p$$

$$= \{T/(p+1)\}(h/2)^p.$$

Therefore $\|K\|_{L(p)} = \{T/(p+1)\}^{1/p}(h/2)$. Since

$$\int_0^T |t^{-1/2}|^q dt = \{2/(2-q)\}T^{1-q/2},$$

then

$$|E(T)| \leq (1/4)\{T/(p+1)\}^{1/p}\{2/(2-q)\}^{1/q}T^{1/q - 1/2}$$

$$= T^{1/2}(p+1)^{-1/p}\{2/(2-q)\}^{1/q}(h/4).$$

One could proceed further and analyze the constant

$$k(q) = (p+1)^{-1/p}\{2/(2-q)\}^{1/q}$$

subject to $1/p + 1/q = 1$, $1 \leq q < 2$. One can conclude (by very tedious manipulations) that $k(q)$ for $1 \leq q < 2$ takes on its minimum at $q = 1$. In this case $k(1) = 2$. Hence the minimum estimate on $|E(T)|$ by this application of the Minkowski inequality to Peano's theorem is

$$|E(T)| \leq (\sqrt{T}\, h)/2.$$

Although this estimate is optimal (in the above sense), it is overly pessimistic, because one can show that $E(T) = \mathcal{O}(h^{3/2})$. This can be seen in Example 2 in Section 3 below. Indeed with a little extra care one can sharpen the result in Example 2 to show that

$$1/6 \leq h^{-3/2} E(T) \leq 1/6 + 1/16.$$

This then clearly demonstrates that applying the Minkowski inequality to Peano's theorem may possibly yield substantially less information than is desirable.

In Section 2 we shall show how Peano's theorem and the Minkowski inequality can be applied in general to singular quadrature questions. In particular we generalize the first type of analysis presented above for $\int_0^T t^{1/2} dt$ where $E(T) = \mathcal{O}(h)$. In Section 3 we shall refine our analysis to obtain better information. In particular we generalize the second type of analysis stated above forthe case $\int_0^T t^{1/2} dt$ where $E(T) = \mathcal{O}(h^{3/2})$.

The drawbacks for the usual Minkowski-Peano approach become even more exaggerated for $\int_0^T t^{-1/2} dt$ where the integrand itself has a weak singularity. Since the hypotheses of Peano's theorem requires absolute continuity and since $f(t) = t^{-1/2}$ is not even continuous at zero, then Peano's theorem cannot be applied directly. In Section 4 we show how this situation can be remedied. We propose a simple modification of the usual compound quadrature rule which we call the method of "avoiding the singularity". We then establish general error bounds along with convergence rates for this numerical quadrature of weakly singular integrands.

The use of Peano's theorem to obtain error estimates for quadrature of functions with low continuity is known. For example Stroud [2] has recently studied certain aspects of this method. Numerical quadrature of singular functions has also been studied. Davis and Rabinowitz [3] establish various convergence theorems with interesting lim inf results which were extended by Rabinowitz [4]. Gautschi [5] applied some of the work of Rabinowitz and obtained convergence theorems for two quadratures of interpolatory type. In none of these papers are error bounds explicitly given, although for example the proofs in [2] may be used to obtain certain estimates (see [2], line (3.7) and the proof of Theorem 3). All of these results require that the integrand be monotone in a neighborhood of the singularity. Fox [6] gives some error bounds for singular quadratures. His work is very special and does not seem to generalize.

The main results of this paper predict rather slow convergence rates for weakly singular numerical quadratures. Various numerical experiments verify these predictions. Moreover there may be no advantage in using a better rule (e.g. Simpson rather than trapazoid), see [7, p. 77] for a striking example of this. If one knows enough about the integrand, it may be possible to change variables or otherwise to eliminate the singularity, see for example [7, pp. 72-73] or [8, pp. 346-352]. In other cases one might wish to use special numerical quadrature methods which are specifically designed for particular singular integrands. Two examples of such methods are given in Atkinson [9, sections 2.1 and 2.2] and Schweikert [10].

In Section 5 we apply our results of the earlier sections to the question of singular quadrature in the convolution case. This work in particular will be used in its full generality by the authors in a sequel paper which studies numerical solution of weakly singular Volterra integral equations of the form

$$x(t) = f(t) + \int_0^t a(t-s)G(x(s))ds \quad (0 \le t \le T)$$

where f and G are smooth but $a(t)$ may be singular at $t = 0$; $(a(t) = t^{-1/2})$.

2. Basic Estimates

Consider an approximate quadrature rule defined on the standard interval $0 \le t \le 1$:

(R) $$R(f) = \sum_{j=0}^{J} w_j f(x_j)$$

with error

$$E(f,R) = \int_0^1 f(t)dt - R(f).$$

It will always be assumed that the abscissas x_j satisfy the inequalities $0 \leq x_0 < x_1 < \ldots < x_J \leq 1$. In addition we shall assume some or all of the following hypotheses in the sequel:

(A1) $f \in C^{n-1}[0,1]$ where $n \geq 1$ is a fixed integer and $f^{(n-1)}$ is absolutely continuous on $0 \leq t \leq 1$.

(A2) $E(p,R) = 0$ for all polynomials $p(t)$ of degree $\leq n-1$.

(A3) The weights w_j are positive for $j = 0(1)J$.

(A4) $f \in C^{n-1}[0,T]$ and $f^{(n-1)}$ is absolutely continuous on $[0,T]$.

The symbols $j = 0(1)J$ means $j = 0,1,2,\ldots,J$. The integer $n \geq 1$ in hypotheses (A1) and (A2) are the same fixed value.

For any subinterval I of the real line let $\chi_I(t)$ denote the characteristic function of the interval I, that is

$$\chi_I(t) = 1 \text{ if } t \in I; = 0 \text{ if } t \notin I.$$

For our purposes the following special case of Peano's theorem will suffice, c.f. [1, p. 14].

Theorem 1. *Assume the rule* (R) *together with hypotheses* (A1) *and* (A2). *Define*

$$f_s(t) = (t-s)^{n-1}\chi_{[0,s]}(t)/(n-1)!$$

for $0 \le s,t \le 1$ *where* n *is the integer given in* (A1-2). *Then the error* $E(f,R)$ *may be written in the form*

$$E(f,R) = \int_0^1 f^{(n)}(s)K_n(s)ds \tag{1}$$

where $K_n(s) = -E(f_s,R)$ *for* $0 \le s \le 1$.

The function $K_n(s)$ can be explicitly calculated when R and n are known. For example if R is the midpoint rule, then $J = 0$, $w_0 = 1$ and $x_0 = 1/2$. For $n = 1$

$$K_1(s) = -s \text{ if } 0 \le s < 1/2; = 1-s \text{ if } 1/2 \le s < 1.$$

In the general case

$$K_n(s) = (-1)^n s^n/n! + \sum_{j=0}^{k} w_j(x_j-s)^{n-1}/(n-1)! \tag{2}$$

when $x_k \le s < x_{k+1}$. If $x_0 > 0$ or if $x_J < 1$, then similiar formulas may be obtained for the intervals $0 \le s < x_0$ and $x_J \le s < 1$. In particular (2) shows that K_n is of class $L^p(0,1)$ for all numbers p in the interval $1 \leq p \leq \infty$. Therefore Theorem 1 and the Minkowski inequality imply the following result.

Corollary 1. *Assume the hypotheses of Theorem 1. If* $f^{(n)} \in L^q(0,1)$ *and if* $1/p + 1/q = 1$ *then*

$$|E(f,R)| \leq \{\int_0^1 |K_n(s)|^p ds\}^{1/p} \{\int_0^1 |f^{(n)}(s)|^q ds\}^{1/q} \quad (1 < q < \infty) \tag{3}$$

with similiar formulas for the cases $q = 1$ *and* $q = \infty$.

In general the calculation of the L^p norm

$$\|K_n\|_{L(p)} = \{\int_0^1 |K_n(s)|^p ds\}^{1/p} \quad (1 \leq p < \infty) \tag{4}$$

may be difficult if $1 \leq p \leq \infty$. Since the norm

$$\|K_n\|_{L(\infty)} = \max\{|K_n(s)| : 0 \leq s \leq 1\} \tag{4.1}$$

is easy to obtain numerically, then it may be convenient to use the estimate $\|K_n\|_{L(p)} \leq \|K_n\|_{L(\infty)}$. If this is not sufficient, then it is possible to obtain a universal estimate under the additional hypotheses (A3).

Corollary 1*. *Assume the hypotheses of Theorem 1. If* $f^{(n)} \in L^q(0,1)$ *and* $1/p + 1/q = 1$, *then*

(3') $\quad |E(f,R)| \le \|K_n\|_{L(p)} \|f^{(n)}\|_{L(q)} \le \|K_n\|_{L(\infty)} \|f^{(n)}\|_{L(q)}$.

If in addition (A3) *is true, then* $\|K_n\|_{L(\infty)} \le (n+1)/n!$

Proof. Only the last statement needs further proof. Assumptions (A2) and (A3) imply that $\sum_{j=0}^{J} w_j = 1$. For $k = 0(1)J$ and for s in the interval $x_k \le s < x_{k+1}$ equation (2) implies that

$$|K_n(s)| \le 1/n! + \sum_{j=0}^{k} w_j/(n-1)!$$

$$\le 1/n! + (\sum_{j=0}^{J} w_j)/(n-1)! = (n+1)/n!$$

If $x_0 > 0$ then $|K_n(s)| \le 1/n! \le (n+1)/n!$ in the interval $0 \le s < x_0$. Similiarly if $x_J < 1$ and if $x_J \le s < 1$ then $|K_n(s)| \le (n+1)/n!$. Q.E.D.

These basic results are easily extended to general intervals and to compound rules. Given an interval $a \le t \le a+B$, one can use the transformation $\tau = a+Bt$ to compute

$$\int_a^{a+B} F(\tau)d\tau = B \int_0^1 F(a+Bt)dt \doteq B \sum_{j=0}^{J} w_j F(a+Bx_j).$$

For example if (R) is the midpoint rule $R(f) = f(1/2)$, then one can replace B by h and write

$$\int_a^{a+h} F(\tau)d\tau \doteq h\, F(a+h/2)$$

in the usual way. If (R) is Simpson's Rule, then we think of $B = 2h$ and write

$$\int_a^{a+2h} F(\tau)\,d\tau \doteq (h/3)\{F(a) + 4F(a+h) + F(a+2h)\}.$$

Corollary 2. Assume (A2) is true, $F \in C^{n-1}[a, a+B]$ and $F^{(n-1)}$ is absolutely continuous on $a \leq t \leq a+B$. Then all the following statements are true.

a. The error $E = \int_a^{a+B} F(t)\,dt - B \sum_{j=0}^{J} w_j F(a+Bx_j)$ may be written in the form

$$E = B^n \int_a^{a+B} K_n\left(\frac{s-a}{B}\right) F^{(n)}(s)\,ds$$

where $K_n(s)$ is the function given in Theorem 1 above.

b. If $F^{(n)} \in L^q(a, a+b)$, if $1/p + 1/q = 1$ and if $\|K_n\|_{L(p)}$ is the L^p norm of K_n over the interval $[0,1]$ (see (4)), then

$$|E| \leq B^{n+1/p} \|K_n\|_{L(p)} \{\int_a^{a+B} |F^{(n)}(s)|^q ds\}^{1/q}.$$

c. If in addition to the hypotheses listed above (A3) is also true, then

$$|E| \leq B^{n+1/p} (n+1)/n! \{\int_a^{a+B} |F^{(n)}(s)|^q ds\}^{1/q}.$$

Proof. By Theorem 1 above

$$\begin{aligned} E &= B\int_0^1 F(a+Bt)dt - B\sum_{j=0}^{J} w_j F(a+Bx_j) \\ &= B\int_0^1 K_n(s)\{\frac{d^n}{ds^n}F(a+Ba)\}ds \\ &= B^{n+1}\int_0^1 K_n(s)F^{(n)}(a+Bs)ds \\ &= B^n \int_a^{a+B} K_n(\frac{s-a}{B})F^{(n)}(s)ds. \end{aligned}$$

This proves a. Part b. follows from part a. and change of variables

$$\{\int_a^{a+B}|K_n(\frac{s-a}{B})|^p ds\}^{1/p} = \{\int_0^1 |K_n(s)|^p B\ ds\}^{1/p} = B^{1/p}\|K_n\|_{L(p)}.$$

Part c. follows from b. since $\|K_n\|_{L(p)} \leq \|K_n\|_{L(\infty)} \leq (n+1)/n!$ Q.E.D.

Now consider a compounding of the rule R over an interval $0 \leq t \leq T$. Let $T = NB$ where $B > 0$ and where N is an integer larger than one. If R is compounded N times over $[0,T]$ then

$$(N \times R) \qquad N \times R(f) = \sum_{k=0}^{N-1}\{\sum_{j=0}^{J} Bw_j f(Bx_j+kB)\}.$$

Let $E_N(f) = \int_0^T f(t)dt - N \times R(f)$ be the error.

Corollary 3. <u>Suppose</u> (A2) <u>and</u> (A4) <u>are true. Then all of the following statements are true:</u>

a. $E_N(f) = \int_0^T f^{(n)}(t)\overline{K}_n(t)dt$ <u>where</u> $\overline{K}_n(t) = K_n(t/B - k)$ <u>on</u> $kB \leq t < (k+1)B$.

b. <u>If</u> $f^{(n)} \in L^q(0,T)$, $1/p + 1/q = 1$ <u>and</u> $\|K_n\|_{L(p)}$ <u>is defined as in</u> (4), <u>then</u>

$$|E_N(f)| \leq B^n T^{1/p} \|K_n\|_{L(p)} \{\int_0^T |f^{(n)}(t)|^q dt\}^{1/q}$$

c. <u>If in addition</u> (A3) <u>is true, then</u>

$$|E_N(f)| \leq \{B^n T^{1/p}(n+1)/n!\}\{\int_0^T |f^{(n)}(t)|^q dt\}^{1/q}.$$

Proof. Write the error in the form

$$E_N(f) = \sum_{k=0}^{N-1}\{\int_{kB}^{kB+B} f(t)dt - \sum_{j=0}^{J} Bw_j f(B(x_j+k))\},$$

and then apply Corollary 2.a:

$$E_N(f) = \sum_{k=0}^{N-1} B^n \int_{kB}^{kB+B} f^{(n)}(t) K_n(t/B-k)dt = B^n \int_0^T f^{(n)}(t)\bar{K}_n(t)dt.$$

Since $\bar{K}_n(t)$ is periodic of period B on $0 \leq t \leq T$, then

$$\int_0^T |\bar{K}_n(t)|^p dt = N \int_0^B |\bar{K}_n(t)|^p dt = NB \int_0^1 |K_n(t)|^p dt$$
$$= T\{\|K_n\|_{L(p)}\}^p.$$

Therefore

$$B^{-n}|E_N(f)| \leq \{\int_0^T |f^{(n)}(t)|^q dt\}^{1/q}\{\int_0^T |\bar{K}_n(t)|^p dt\}^{1/p}$$

$$= \{\int_0^T |f^{(n)}(t)|^q dt\}^{1/q} T^{1/p} \|K_n\|_{L(p)}.$$

If (A3) is true then $\|K_n\|_{L(p)} \leq \|K_n\|_{L(\infty)} \leq (n+1)/n!$ Q.E.D.

Example 1. Consider $\int_0^1 t^{1/2} dt$ approximated by the trapezoid rule. In this case $B = h$, $T = Nh = 1$, $n = 1$ and $K_1(s) = (1/2)-s$ on the interval $0 \leq s < 1$. Therefore

$$\int_0^1 |K_1(s)|^p ds = \int_0^1 |1/2 - s|^p ds = \int_0^{1/2} |1/2 - s|^p ds + \int_{1/2}^1 |1/2 - s|^p ds$$

$$= \int_0^{1/2} s^p ds + \int_0^{1/2} s^p ds = 2^{-p}(p+1)^{-1}.$$

Since $f'(t) = (2t^{1/2})^{-1} \in L^q(0,1)$ for $1 \leq q < 2$, then Corollary 3 implies that

(5) $$|E_N(t^{1/2})| \leq h\ 2^{-p}(p+1)^{-1}\{\int_0^1 (2t^{1/2})^{-q} dt\}$$

$$= h\{2^{1/q\ -\ p-1}(p+1)^{-1/p}(2-q)^{-1/q}\}$$

for $1 < q < 2$. If $q = 1$, then

(6) $$|E_N(t^{1/2})| \leq h(1/2)\int_0^1 (2t^{1/2})^{-1} dt = h/2.$$

Part c. of Corollary 3 implies an even more pessimistic estimate $|E_N(t^{1/2})| \leq 2h$. Section 3 will produce estimates which are $\mathcal{O}(h^{3/2})$.

3. Refined Estimates.

Definition 1. *A function* f *is said to be weakly singular of order* ν *if and only if*

a. $f \in C(0,T]$ *if* $\nu = 0$ *or* $f \in C^{\nu-1}[0,T] \cap C^{\nu}(0,T]$ *if* $\nu \geq 1$,

b. *for each* $\epsilon > 0$ *the function* $f^{(\nu)}(t)$ *is absolutely continuous on the interval* $\epsilon \leq t \leq T$, *and*

c. *the function* α_ν *defined by*

$$\alpha_\nu(t,f) = |f^{(\nu)}(T)| + \int_t^T |f^{(\nu+1)}(s)|\,ds \tag{7}$$

is of class $L^1(0,T)$.

For any integer $N \geq 0$ let $WS(\nu)$ denote the set of all functions f which are weakly singular of order ν. For example if $0 < r < 1$ and $T = 1$ then $f(t) = \log t$ and $g(t) = \sin(t^{-r})$ are in $WS(0)$. In these two cases $\alpha_0(t,f) = -\log t$ and $\alpha_0(t,g) \leq t^{-r}$. In general $f(t) = t^{\nu-r}$, $0 < r < 1$, is of class $WS(\nu)$ so that each class $WS(\nu)$ is not empty. The following lemma is an immediate consequence of the definition.

Lemma 1. *If* $f \in WS(\nu)$ *then* $|f^{(\nu)}(t)| \leq \alpha_\nu(t,f)$ *on the interval* $0 < t \leq T$.

Theorem 2. *Suppose* (A2) *is true for some integer* $n = \nu+1$ *where* $\nu \geq 1$. *If* $f \in WS(\nu)$ *then the error* $E_N(f)$ *obtained by applying the compound rule* $(N \times R)$ *satisfies the inequality*

(8) $$|E_N(f)| \le B^{\nu}\int_0^B \alpha_\nu(t,f)dt\{\|K_\nu\|_{L(\infty)} + \|K_{\nu+1}\|_{L(\infty)}\}$$

In particular if (A3) *is also true then*

(9) $$|E_N(f)| \le B^{\nu}(\nu^2+3\nu+3)/(\nu+1)!\{\int_0^B \alpha_\nu(t,f)dt\}.$$

Proof. Write $E = E_N(f)$ in the form

$$E = \{\int_0^B f(t)dt - \Sigma_{j=0}^{J} Bw_j f(Bx_j)\} + \{\int_0^{T-B} f(t+B)dt$$

$$- \Sigma_{k=0}^{N-2} Bw_j f(B(x_j+(k+1)))\}.$$

Apply Corollary 3.b to the first summand with $n = \nu$, $q = 1$ and to the second summand with $n = \nu+1$, $q = 1$:

$$|E| \le B^{\nu}\|K_\nu\|_{L(\infty)}\{\int_0^B |f^{(\nu)}(t)|dt\} +$$

$$B^{\nu+1}\|K_{\nu+1}\|_{L(\infty)}\{\int_0^{T-B}|f^{(\nu+1)}(t+B)|dt\}$$

Now use (7) and Lemma 1:

$$|E| \le B^{\nu}\|K_\nu\|_{L(\infty)}\int_0^B \alpha_\nu(t,f)dt +$$

$$B^{\nu+1}\|K_{\nu+1}\|_{L(\infty)}\{\alpha_\nu(B,f)-\alpha_\nu(T,f)\}.$$

Since $\alpha_\nu(t,f)$ is nonnegative and nonincreasing in t, then

$$B\{\alpha_\nu(B,f)-\alpha_\nu(T,f)\} \le B\alpha_\nu(B,f) \le \int_0^B \alpha_\nu(t, f)dt.$$

Therefore (8) follows. The estimate (9) follows from (8) and the inequality $\|K_n\|_{L(\infty)} \leq (n+1)/n!$ Q.E.D.

Example 2. Consider $\int_0^1 t^{1/2} dt$ approximated by the trapezoid rule. (The same example as at the end of section 2.) Then $B = h$, $T = 1 = Nh$, $n = 2$, $\nu = 1$ and

$$K_1(s) = 1/2 - s, \quad K_2(s) = s(s-1)/2.$$

It is easy to compute $\alpha_1(t) = (1/2)t^{-1/2}$ and $\int_0^h \alpha_1(t)dt = h^{1/2}$. Therefore (8) implies that

$$|E_N(t^{1/2})| \leq h(1/2 + 1/8)h^{1/2} = (5/8)h^{3/2}.$$

Even less computation is required to see that (9) implies

$$|E_N(t^{1/2})| \leq (7/2)h^{3/2}.$$

Either result shows that the error is or order $\mathcal{O}(h^{3/2})$ as $h = 1/N \to 0$. The estimates in section 2 where $\mathcal{O}(h)$.

Theorem 2 above cannot be applied if the integer n in hypotheses (A2) is equal to one but $f \in WS(\nu)$ for some integer $\nu \geq 1$. However such situations are already covered by Corollary 3 above. For example if the midpoint rule M is applied to $f(t) = \sqrt{t}$, then by Corollary 3 the error is $\mathcal{O}(h^{1/2})$. The reverse situation $\nu = 0$ and $n \geq 1$ is more complicated. This situation is the topic of the next section.

4. Estimates when $\nu = 0$.

If $f \in WS(\nu)$ and $\nu = 0$, then $t = 0$ may be an unbounded point of f. In this case the compound rule $(N \times R)$ need not be well defined. Even if $(N \times R)$ is well defined (e.g. if rule R is open at $t = 0$) the previous estimates do not apply. One simple method of handling both of these problems is to avoid the singularity at $t = 0$. This idea leads to the following approximation rule:

Let $T = NB$ where $B > 0$ and $N > 1$ is an integer. Compute

$$R_A(T,f) = \sum_{k=1}^{N-1}\{\sum_{j=0}^{J} Bw_j f(x_j B+kB)\}$$

and let $E_A(f,N)$ = error.

Rule R_A will be called the method of "avoiding the singularity". This rule is the usual compound rule except that no attempt is made to approximate on the initial segment $[0,B]$.

Theorem 3. <u>Suppose</u> (A2) <u>is true for</u> $n = 1$. <u>If</u> $f \in WS(0)$ <u>then</u>

$$(10) \qquad |E_A(f,N)| \leq \{1 + \|K_1\|_{L(\infty)}\}\int_0^B \alpha_0(t,f)dt.$$

<u>In particular if</u> (A3) <u>is also true, then</u>

$$(11) \qquad |E_A(f,N)| \leq 3 \int_0^B \alpha_0(t,f)dt.$$

Proof. Define $f_B(t) = f(t+B)$ on $0 \le t \le T-B$. Then the error $E_A = E_A(f,N)$ has the form

$$E_A = \int_0^B f(t)dt + E_{N-1}(f_B)$$

where $E_k(g)$ is error for the usual compound rule. Apply Corollary 3.b with $n = q = 1$:

$$|E_A| \le \int_0^B |f(t)|\,dt + B\|K_1\|_{L(\infty)}\int_0^{T-B}|(f_B)'(t)|\,dt$$
$$= \int_0^B |f(t)|\,dt + B\|K_1\|_{L(\infty)}\int_B^T |f'(t)|\,dt.$$

Use Lemma 1 and the definition (7):

$$\int_0^B |f(t)|\,dt \le \int_0^B \alpha_0(t,f)dt,$$

and

$$\int_B^T |f'(t)|\,dt = \alpha_0(B,f) - \alpha_0(T,f)$$
$$\le (1/B)B\alpha_0(B,f) \le (1/B)\int_0^B \alpha_0(t,f)dt.$$

This proves (10).

If (A3) is also true, then $\|K_1\|_{L(\infty)} \le (1+1)/1! = 2$. Therefore (11) follows immediately from (10). Q.E.D.

Example 3. If $f(t) = t^{-r}$, $0 < r < 1$, then it is easy to compute $\alpha_0(t,f) = t^{-r}$. Theorem 3 predicts $E_A = \mathcal{O}(B^{1-r})$ as $B \to 0$. If $f(t) = t^{-r}\sin(t^{-\nu})$, where $r,\nu > 0$ and $r+\nu < 1$, then by Theorem 3 one has at least $E_A = \mathcal{O}(B^{1-r-\nu})$. If $f(t) = t^{-r}\sin(\log t)$ where $0 < r < 1$ then $E_A = \mathcal{O}(B^{1-r})$ at least.

5. Convolution Integrals

Consider a convolution integral

$$I = \int_0^T f(T-s)g(s)ds = \int_0^T f(s)g(T-s)ds. \tag{12}$$

Theorem 4. Suppose (A2) is true for $n = \nu+1$. In addition assume

i. $f \in WS(\nu)$ where $\nu \geq 1$ and

ii. $g \in C^{\nu}[0,T] \cap C^{\nu+1}(0,T]$ with $g^{(\nu+1)} \in L^1(0,T)$.

Define $F(t) = f(t)g(T-t)$ on $0 \leq t \leq T$. Let $L > 0$ be a bound for each of the functions $|f(t)|$, $|g(t)|$, $|g'(t)|,\ldots,|g^{(\nu)}(t)|$ on the interval $0 \leq t \leq T$. Then the error $E_N(F)$ obtain by applying the compound rule $N \times R$ to F satisfies the estimate

$$|E_N(F)| \leq LB^{\nu}(\|K_\nu\|_{L(\infty)} + \|K_{\nu+1}\|_{L(\infty)})\{\int_0^B \alpha_\nu(t,f)dt$$
$$+ B\int_0^T(|g^{(\nu+1)}(s)| + \Sigma_{j=1}^{\nu}\binom{\nu+1}{j}|f^{(j)}(s)|)ds\}$$

where $\binom{k}{j} = k!/j!(k-j)!$.

Proof. For any number s in the interval $0 < s \le T$ one has

$$F^{(\nu+1)}(s) = \sum_{j=0}^{\nu+1}(-1)^j\binom{\nu+1}{j}f^{(\nu+1-j)}(s)g^{(j)}(T-s).$$

Therefore if L is the bound defined above, then

$$|F^{(\nu+1)}(s)| \le L\{\sum_{j=0}^{\nu}\binom{\nu+1}{j}|f^{(\nu+1-j)}(s)|\} + L|g^{(\nu+1)}(T-s)|.$$

This shows that $F \in WS(\nu)$ and

$$\alpha_\nu(t,F) \le L\alpha_\nu(t,f) + L\int_t^T\{g^{(\nu+1)}(T-s) + \sum_{j=1}^{\nu}\binom{\nu+1}{j}|f^{(j)}(s)|\}ds.$$

Apply Theorem 2:

$$|E_N(F)| \le B^\nu(\|K_\nu\| + \|K_{\nu+1}\|)\int_0^B\alpha_\nu(t,F)dt$$

$$\le LB^\nu(\|K_\nu\| + \|K_{\nu+1}\|)\{\int_0^B\alpha_\nu(t,f)dt + \int_0^B\int_t^T(|g^{(\nu+1)}(T-s)| + \sum_{j=1}^{\nu}\binom{\nu+1}{j}|f^{(j)}(s)|)dsdt\}.$$

By nonnegativity and Fubini's theorem

$$\int_0^B\int_t^T(|g^{(\nu+1)}(T-s)| + \sum_{j=1}^{\nu}\binom{\nu+1}{j}|f^{(j)}(s)|)dsdt$$

$$\le \int_0^B\int_0^T(\ldots)dsdt = \int_0^T\int_0^B(\ldots)dtds$$

$$= B\int_0^T(|g^{(\nu+1)}(s)| + \sum_{j=1}^{\nu}\binom{\nu+1}{j}|f^{(j)}(s)|)ds. \quad \text{Q.E.D.}$$

The next results follow immediately from Theorem 4.

Corollary 4. *Suppose the hypotheses of Theorem 4 are true. Pick any number* $M_1 > 0$ *which satisfies the estimate*

$$b \le M_1 \int_0^b \alpha_\nu(t,f)dt. \quad (0 < b \le T)$$

Then $|E_N(F)| \le MB^\nu\int_0^B\alpha_\nu(t,f)dt$ *where*

(14) $$M = L(\|K_\nu\|_{L(\infty)} + \|K_{\nu+1}\|_{L(\infty)})(1 + M_1\int_0^T(|g^{(\nu+1)}(s)| + \sum_{j=1}^{\nu}\binom{\nu+1}{j}|f^{(j)}(s)|)ds).$$

Corollary 5. *Suppose the hypotheses of Theorem 4 are true. For any integer* $N > 0$ *let* $B = T/N$ *and define*

$$I_j = \int_0^{jB} f(s)g(jB-s)ds. \quad (j = 1(1)N)$$

Let E_j *be the error in approximating* I_j *by the compound rule* $(j \times R)$. *Then*

$$|E_j| \leq MB^{\nu}\int_0^B \alpha_\nu(t,f)dt \quad (j = 1(1)N)$$

where M *is the constant defined by* (14). *In particular* M *is independent of* $N \geq 1$ *and of* $j = 1(1)N$.

A similar analysis obtains when $\nu = 0$.

Theorem 5. *Suppose* (A2) *is true for* $n = 1$. *Assume* $f \in WS(0)$, g *is absolutely continuous on* $0 \leq t \leq T$ *and* L *is a bound on* $|g(t)|$ *for* $0 \leq t \leq T$. *Define*

$$F(s) = f(s)g(T-s) \quad (0 < t \leq T).$$

Then the error E_A *obtained by applying the method avoiding the singularity to* F *satisfies the estimate*

$$|E_A(f,N)| \leq (1 + \|K_1\|_{L(\infty)})(L + \int_0^T |g'(s)|ds)\int_0^B \alpha_0(t,f)dt.$$

Proof. Since $F'(s) = f'(s)g(T-s)-f(s)g'(T-s)$, then $F \in WS(0)$ and

$$\begin{aligned}|F'(s)| &\leq L|f'(s)| + |f(s)||g'(T-s)| \\ &\leq L|f'(s)| + \alpha_0(s,f)|g'(T-s)|\end{aligned}$$

on $0 < s < T$. In particular then

$$\alpha_0(t,F) \leq L\alpha_0(t,f) + \int_t^T \alpha_0(s,f)|g'(T-s)|ds.$$

Apply Theorem 3:

$$|E_A| \le (1 + \|K_1\|)\int_0^B \alpha_0(t,F)dt$$

$$\le (1+\|K_1\|)(L\int_0^B \alpha_0(t,f) + \int_0^B\int_t^T \alpha_0(s,f)|g'(T-s)|dsdt.$$

Since $\alpha_0(t,f)$ is nonnegative and monotone in t, then

$$\int_0^B\int_t^T \alpha_0(s,f)|g'(T-s)|dsdt \le \int_0^B \alpha_0(t,f)\int_t^T |g'(T-s)|dsdt$$

$$\le (\int_0^B \alpha_0(t,f)dt)(\int_0^T |g'(s)|ds). \quad \text{Q.E.D.}$$

Corollary 6. <u>Assume the hypotheses of Theorem</u> 5. <u>For any integer</u> $N > 0$ <u>let</u> $B = T/N$ <u>and define</u>

$$I_j = \int_0^{jB} f(s)g(jB-s)ds. \quad (j = 1(1)N)$$

<u>Let</u> $E_A(j)$ <u>be the error obtained in approximating</u> I_j <u>by the rule</u> R_A. <u>Then</u>

$$|E_j| \le (1 + \|K_1\|_{L(\infty)})(L + \int_0^T |g'(s)|ds)\int_0^B \alpha_0(t,f)dt$$

<u>where</u> L <u>is the bound defined in Theorem</u> 5. (<u>This estimate is independent of</u> N <u>and</u> j.)

5. Numerical Examples.

The results in sections 3 and 4 were verified by numerically integrating the function $f(t) = \alpha t^a \sin(t^{-b})$ for various values of the parameters α, a and b with $-1 < a < 1$ and $0 \leq b < 1$. These computations were performed on a CDC 6600 computer at the Lawrence Radiation Laboratory, U.S. Atomic Energy Commission. They were designed and implemented with the help of Dr. Fred Fritsch.

Some computations were recomputed in double precision. The numerical evidence obtained in this way suggests that round off errors had no effects on the calculations over the full range of values of h. Experiments were made using both the method of "ignoring" the singularity (see [3]) and the method of "avoiding" the singularity (section 3 above). "Avoiding" is easier to handle theoretically while "ignoring" was a bit easier to program. Ignoring gives slightly better accuracy for monotone integrands while avoiding may be a bit better for oscillating integrands.

Table 1 contains results for the integral

$$I = (1+a)\int_0^1 t^a dt = 1, \tag{15}$$

for the value $a = -1/4$. Simpson's rule was employed with $h = 2^{-k}$ and $k = 1(1)15$. The constants $C(h)$ in table 1 were computed by putting the error in the form $E(h) = C(h)h^{1+a}$. Then

(16) $$C(h) = E(h)/h^{1+a}.$$

These values of $C(h)$ appear to be converging as $h \to 0$. As a second check on the possible asymptotic form of the error one can assume that $E(h) = C_0 h^\rho$ (at least asymptotically). Then ρ may be calculated using the formulas

(17) $$Q = \frac{E(h) - E(2h)}{E(h/2) - E(h)}, \quad \rho = \frac{\log Q}{\log 2}.$$

(One can also calculate C_0 in this manner.) The last column in table 1 is computed using (17).

(Printer: Insert table 1 near here)

Table 1 indicates slow but monotone convergence. The error appears to have the form $E(h) = C(h)h^{3/4}$ where $C(h) \to C_0 = .60996...$ as $h \to 0$. This general behavior is typical of the integrand (15) for $0 < |a| < 1$. For example if $a = .75$ in (15) Simpson's rule gives much more rapid monotone convergence:

$$S(2^{-5}) = .99956,$$

$$S(2^{-10}) = .99999\,88,$$

$$S(2^{-15}) = .99999\,9997.$$

In $E(h) = C(h)h^{1.75}$ the corresponding values of $C(h)$ are:

$$C(2^{-5}) = -.1878,$$

$$C(2^{-10}) = -.2145,$$

$$C(2^{-15}) = -.2265.$$

The values of $C(h)$ appear to be converging rather slowly. If $a = -.99$ in (15), then Simpson's rule hardly appears to converge at all:

$$S(2^{-5}) = .039,$$

$$S(2^{-10}) = .072,$$

$$S(2^{-15}) = .104.$$

On the other hand the constant $C(h)$ in the error term converges rapidly:

$$C(2^{-1}) = -.994438,$$

$$C(2^{-2}) = -.994287,$$

$$C(2^{-3}) = -.994284,$$

$$C(2^{-4}) = -.994238$$

$$C(2^{-5}) = -.99423\ 596$$

$$C(2^{-6}) = -.99423\ 534$$

and

$$C(2^{-k}) = -.99423\,5131 \quad \text{for} \quad k = 10(1)15.$$

(Printer: Insert Table 2 near here)

Table 2 contains results (using the trapezoid rule) for the integral

$$I = \int_0^1 t^{-1/2} \sin(t^{-b})dt$$

where $b = .25$. Convergence is very slow and is not monotone. No asymptotic formula $E(h) \approx C_0 h^\rho$ is discernible using either of the two tests (16) and (17). On the other hand for the small value $b = .01$ convergence is monotone at a rate $E(h) = C(h)h^{.49}$ where $C(h)$ is a slowly varying function of h:

$$C(2^{-1}) = 1.286,$$

$$C(2^{-5}) = 1.246,$$

$$C(2^{-10}) = 1.228.$$

At the opposite extreme $b = .49$ convergence is very slow

$$T(2^{-5}) = .9477,$$

$$T(2^{-10}) = .9972,$$

$$T(2^{-15}) = 1.0232,$$

convergence is not monotone and no approximate asymptotic error formula is apparent.

Table 1: $f(t) = .75t^{-.25}$

k	Error	C	ρ
1	-.36655	-.61645	
2	-.21663	-.61271	
3	-.12847	-.61112	.76609
4	-.07631	-.61045	.75692
5	-.04535	-.61016	.75293
6	-.02696	-.61005	.75123
7	-.01629	-.61000	.75052
8	-.00953	-.60997	.75022
9	-.00567	-.60995	.75009
10	-.00337	-.60996	.75004
11	-.00200	-.60996	.75002
12	-.00119	"	.75001
13	-.00071	"	.75000
14	-.00042	"	"
15	-.00025	"	"

Table 2: $f(t) = t^{-1/2}\sin(t^{-1/4})$

k	$2^k \times T$	k	$2^k \times T$	k	$2^k \times T$
1	.8666	6	1.5951	11	1.5103
2	1.1810	7	1.5696	12	1.5211
3	1.3948	8	1.5319	13	1.5157
4	1.5252	9	1.5034	14	1.5102
5	1.5867	10	1.4975	15	1.5164

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